Approximate analysis and design of rectangular-lattice photonic crystals

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We present a theoretical analysis of wave propagation in rectangular- and square-lattice photonic crystals by approximating the arbitrary refractive-index function with a staircase profile. This profile has a number of tunable parameters that allow one to fit the band structures of the staircase and the desired structure over a large frequency range. The staircase profile is such that its corresponding two-dimensional wave equation decomposes into two one-dimensional equations by means of a constant decoupling parameter. We show that basic features of the band structure and Bloch waves in photonic crystals can be analyzed theoretically through this simple approximation.

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Computation of band structure in two-dimensional (2D) photonic crystals (PCs) is usually done with extensive numerical simulation techniques such as plane-wave expansion[1] (PWE) and finite-difference time-domain simulations.[2] The PWE approach needs eigenvalue computation of large nonsparse matrices, and the finite-difference time-domain simulations are also capable of calculating the partial band. Another existing method, namely, the transfer matrix method,[3] is also based on expansion on plane waves. Stable and more-efficient numerical methods based on multiple multipole expansion derived from scattering matrices,[4] impedance matrices,[5] and a finite-element method[6] have also been reported. Recently a method of moments was also used in analysis of PC structures.[7] Whereas all these methods are accurate enough, their extensive numerical nature limits their usefulness for perceptive, and therefore approximate, understanding of underlying physics.

In this Letter we present a simple approach to the analysis of propagation of light in PCs. The motivation for this study came from the theory of one-dimensional (1D) electronic crystals and PCs, in which a simple stepwise profile can explain basic phenomena such as electron and photon effective mass, group velocity, and forbidden bands.[8] We therefore consider a periodic staircase profile in the x-y plane with orthogonal periodicity axes and a separable permittivity profile as a sum of functions of x and y alone. The descriptive wave equation for such a structure can be immediately decoupled into two 1D equations. Thus the analysis of a propagation problem in two dimensions reduces to the solution of two 1D systems. The staircase profile has a number of tunable parameters with which one can match the first few x and y harmonics of the desired and staircase structures. We show that through this approach the band structure of a rectangular-lattice PC can be easily reproduced from a properly fitted staircase structure. We present a theoretical analysis of the staircase structure, obtain analytical expressions for the band structure, and show that the results are in agreement with PWE calculations.

The staircase-approximating permittivity profile of a square- or rectangular-lattice PC as shown in Fig. 1 is given by

$$\epsilon(x,y) = \chi(x) + \psi(y)\,, \tag{1}$$

in which $\chi(x)$ and $\psi(y)$ are the periodic staircase profiles

$$\chi(x) = \epsilon_a + [u(x + 1/2\,t) - u(x - 1/2\,t)](\epsilon_b - \epsilon_a)$$
$$|x| \le 1/2\,X\,, \quad \chi(x) = \chi(x + mX)\,, \tag{2a}$$
$$\psi(y) = \epsilon_c + [u(y + 1/2\,s) - u(y - 1/2\,s)](\epsilon_d - \epsilon_c)$$
$$|y| \le 1/2\,Y\,, \quad \psi(y) = \psi(y + nY)\,, \tag{2b}$$

where $u()$ is the Heaviside unit-step function, X and Y are the spatial periods along the x and y directions, m and n are integers, $t < X$ and $s < Y$ are positive constants that determine the widths of the step peaks, and ϵ_j, $j = a, b, c, d$ are dimensionless constants. One can use ϵ_j, t, and s as tunable parameters to obtain the best fit to the band structure of a desired PC, as described below. For the moment, we limit our attention to transverse modes that have electric fields perpendicular to the periodicity plane (TE modes).

The 2D wave equation for TE modes reads as

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)A(x,y) + \frac{\omega^2}{c^2}\,\epsilon(x,y)A(x,y) = 0\,, \tag{3}$$

where $A(x,y)$ is the local amplitude of the transverse electric field, c is the speed of light in vacuum, and ω is

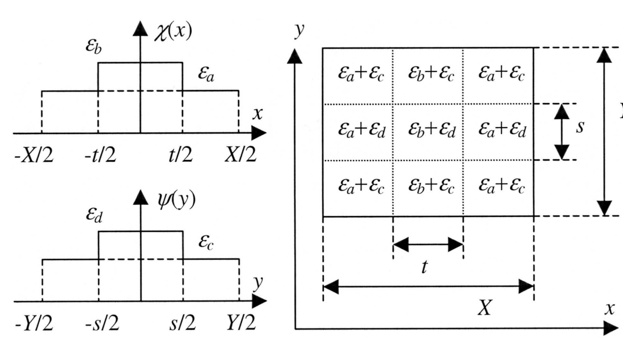

Fig. 1. Staircase approximation of Fig. 1: profiles of $\chi(x)$ and $\psi(y)$ functions as given by Eq. (2) and the corresponding 2D unit cell.

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the angular frequency. For $\epsilon(x, y)$ given by Eq. (1), it is possible to decompose Eq. (3) into two 1D differential equations as

$$\frac{\partial^2}{\partial x^2}\Lambda(x) + \frac{\omega^2}{c^2}[\chi(x) + \beta]\Lambda(x) = 0\,, \tag{4a}$$

$$\frac{\partial^2}{\partial y^2}\Psi(y) + \frac{\omega^2}{c^2}[\psi(y) - \beta]\Psi(y) = 0\,, \tag{4b}$$

where β is a separation constant and $A(x, y) = \Lambda(x)\Psi(y)$. Because the functions $\chi(x) + \beta$ and $\psi(y) - \beta$ are also periodic with periods X and Y, respectively, Eqs. (4a) and (4b) have Bloch-like solutions, given as $\Lambda(x) = \Delta_\kappa(x)\exp(-j\kappa x)$ and $\Psi(y) = \Theta_\eta(y)\exp(-j\eta y)$, where $\Delta_\kappa(x) = \Delta_\kappa(x + mX)$, $\Theta_\eta(y) = \Theta_\eta(y + nY)$, and κ and η are Bloch wave numbers found from the well-known x and y dispersion equations[9]

$$\cos(\kappa X) = \frac{q_{11}}{2}\exp\left\{-j\omega\frac{X}{c}[\chi(-{}^1\!/_2 X) + \beta]^{1/2}\right\} + \frac{q_{22}}{2}\exp\left\{+j\omega\frac{X}{c}[\chi(-{}^1\!/_2 X) + \beta]^{1/2}\right\}, \tag{5a}$$

$$\cos(\eta Y) = \frac{p_{11}}{2}\exp\left\{-j\omega\frac{Y}{c}[\psi(-{}^1\!/_2 Y) - \beta]^{1/2}\right\} + \frac{p_{22}}{2}\exp\left\{+j\omega\frac{Y}{c}[\psi(-{}^1\!/_2 Y) - \beta]^{1/2}\right\}. \tag{5b}$$

Here, q_{ii} and p_{ii} are the diagonal elements of the transfer matrices of the periods $|x| \le {}^1\!/_2 X$ and $|y| \le {}^1\!/_2 Y$, respectively.[9] These equations can be simplified as

$$\cos(\kappa X) = \cos(k_b t)\cos[k_a(X - t)] - \frac{k_a{}^2 + k_b{}^2}{2k_a k_b}\sin(k_b t)\sin[k_a(X - t)], \tag{6a}$$

$$\cos(\eta Y) = \cos(k_d s)\cos[k_c(Y - s)] - \frac{k_c{}^2 + k_d{}^2}{2k_c k_d}\sin(k_d s)\sin[k_c(Y - s)], \tag{6b}$$

in which $k_j = c^{-1}\omega\sqrt{\epsilon_j + \beta}$, $j = a, b, c, d$. The set of Eqs. (6) has parametric solutions in the form $\kappa = \kappa(\omega, \beta)$ and $\eta = \eta(\omega, \beta)$, so one can easily compute the exact band structure.

Now consider the arbitrary periodic profile $f(x, y) = f(x + mX, y + nY)$ with the Fourier series expansion and the Fourier coefficients f_{mn}:

$$f(x, y) = \sum_m \sum_n f_{mn}\exp\left[j2\pi\left(m\frac{x}{X} + n\frac{y}{Y}\right)\right], \tag{7a}$$

$$f_{mn} = \frac{1}{XY}\iint_{\text{unit cell}} f(x, y) \times \exp\left[-j2\pi\left(m\frac{x}{X} + n\frac{y}{Y}\right)\right]\mathrm{d}x\mathrm{d}y\,, \tag{7b}$$

where the double integration is taken over a unit cell area. To approximate the arbitrary profile we choose the parameters of the staircase profile (i.e., t, s, and ϵ_i, $i = a, b, c, d$) such that both profiles have the same first three harmonics. The reason for this choice is that all square- or rectangular-lattice PCs must be equivalent as long as their profiles have the same spatial spectrum. In the low- to mid-frequency range, only couplings between lower-order harmonics are important, and the contributions of higher-order harmonics can be neglected. Below, we observe that numerical results justify this point.

Symmetry considerations for square-lattice PCs require that $f_{mn} = f_{nm}$, $f_{0\overline{n}} = \overline{f}_{0n}$, and $f_{\overline{m}0} = \overline{f}_{m0}$, where the bars on subscripts and on the harmonic represent negative and complex conjugates, respectively. Applying the symmetry conditions to the approximate staircase profile results in $t = s$, $\epsilon_a = \epsilon_c$, and $\epsilon_b = \epsilon_d$. The staircase profile has a Fourier expansion given by

$$\chi(x) + \psi(y) = \left(1 - \frac{t}{X}\right)\epsilon_a + \frac{t}{X}\epsilon_b + \left(1 - \frac{s}{Y}\right)\epsilon_c + \frac{s}{Y}\epsilon_d + \frac{2}{\pi}(\epsilon_b - \epsilon_a)\sum_{m>0}\frac{\sin[\pi m(t/X)]}{m} \times \cos\left(2\pi m\frac{x}{X}\right) + \frac{2}{\pi}(\epsilon_d - \epsilon_c)\sum_{n>0}\frac{\sin[\pi n(s/Y)]}{n} \times \cos\left(2\pi n\frac{y}{Y}\right). \tag{8}$$

Therefore it is possible to set up three algebraic equations to match the first three nonzero harmonics of the two structures. Solution of these algebraic equations for a lossless even-symmetric square-lattice PC results in

$$t = \frac{X}{\pi}\cos^{-1}\left(\frac{\Re\{f_{20}\}}{\Re\{f_{10}\}}\right), \qquad \epsilon_a = \frac{f_{00}}{2} - \frac{\pi t\Re\{f_{10}\}}{X\sin(\pi t/X)},$$
$$\epsilon_b = \epsilon_a + \frac{\pi\Re\{f_{10}\}}{\sin(\pi t/X)}. \tag{9}$$

Here $\Re\{\}$ denotes the real-part operator. The fact that lower-order harmonics determine the long-wavelength behavior is justified by another detailed analysis,[10] which shows that the average permittivity, which here is the f_{00} term, must be the effective permittivity in the long-wavelength range of TE modes as well.

To illustrate the method, we choose a 2D square-lattice PC ($X = Y = L$) with Si rods in air ($\epsilon_{\text{air}} = 1$, $\epsilon_{\text{Si}} = 11.4$, $r = 0.40L$), where r is the radius of the rods. For this structure the fitting values are found from Eqs. (9) to be $\epsilon_a = \epsilon_c = -1.0528$, $\epsilon_b = \epsilon_d = 5.7947$, and $t = s = 0.6086L$. The band structure of this PC along the principal directions is plotted in Fig. 2(a). Figures 2(b) and 2(c) show the constant-frequency contours in the 2D plane of the Bloch wave vector ($\kappa-\eta$ plane) for the first two allowed bands of the same PC. Here the solid and dotted curves in Fig. 2 correspond to PWE computations and analytical formulas (5), respectively, for the approximate staircase structure. The band structures of the approximate and original profiles agree

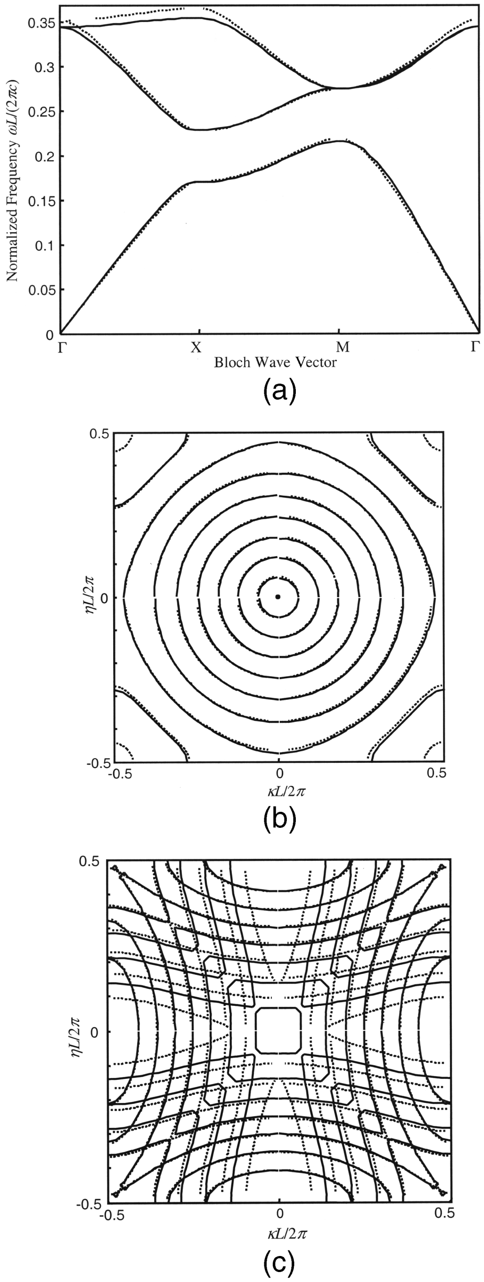

Fig. 2. Structure for TE modes (electric field normal to the plane of periodicity) of allowed bands of the square-lattice PC of Si rods ($r = 0.4L$, where L is the lattice constant). Solid curves, original profile of Fig. 1 computed by the PWE; dotted curves, staircase profile of Fig. 2 computed from analytical expressions given by Eqs. (6a) and (6b). (a) Band structure along high-symmetry directions, (b) constant-frequency contour map of the first band, (c) constant-frequency contour map of the second band.

within 3% up to the normalized frequency $\omega_n = 0.30$. The accuracy of the staircase approximation in the frequency range $0.3 < \omega < 0.35$ is still better than 5%, and it becomes worse for larger frequencies. In fact, $\omega_n = 0.30$ corresponds to the wavelength that satisfies $\lambda_{\text{Si}} = \lambda / n_{\text{Si}} \sim L$, where λ_{Si} and n_{Si} are the wavelength in Si and the refractive index of Si, respectively, and λ is the free-space wavelength. Hence this approximation is reasonable as long as $\lambda_{\text{Si}} > L$. Note that, in the staircase approximation, negative values for permittivity constants ϵ_i, $i = a, b, c, d$, though they are physically not meaningful, are allowed.

The computation time for PWE results was $\sim$10 min when 225 harmonics were used and $\sim$1 min for 100 harmonics (which results in a small computation error), whereas the approximate analytical results from Eq. (6) were computed in just a few seconds. This significant difference between the computation times arises from the fact that we are solving a 1D rather than a 2D problem. Another advantage of the staircase profile is that its band structure is expressed by analytic formulas. We reiterate that the proposed method offers design-oriented formulas with reasonable accuracy for study of the effects of various design parameters on the band structure in practical applications, rather than precise numerical simulation of PC structures.

In conclusion, we have presented a simple approximate approach to the study and design of square- and rectangular-lattice photonic crystals. The method is based on utilizing an approximate staircase permittivity profile with tunable parameters, resulting in a separable 2D wave equation. The method provides a means for derivation of analytic expressions for the Bloch waves and band structure. We showed that the rectangular-lattice PC behaves essentially in the same way as a simple staircase PC, provided that the first few harmonics of the PCs coincide.

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